

PROTOCOL

Groundwater Modeling in the RCRA/CERCLA Process

Introduction

The following protocol has been developed to provide guidance for groundwater modeling for the Savannah River Site Environmental Restoration Program. This protocol is intended to provide guidance that will promote consistency in the application of groundwater modeling in the Work Plan, RFI/RI/BRA, and CMS/FS stages of the RCRA/CERCLA process. The objective is to develop a technically defensible and accurate modeling tool during the RFI/RI/BRA stage for predicting contaminant plume configurations in the future (rather than a snap shot in time), use the model to assess the need for early action, and then evaluate the proposed remedial strategies during the CMS/FS stage.

Details

Work Plan Stage

The need for groundwater modeling should be evaluated early in the RCRA/CERCLA process beginning with the Work Plan stage. Input from the modeling lead should be solicited at this time. Evaluating potential modeling needs at the Work Plan stage will allow for the collection of the necessary data and will reduce the uncertainty in model predictions. Therefore, the quality and quantity of these data must be sufficient for construction of a model that responds in a manner that is consistent with the physical system.

RFI/RI/BRA Stage

Groundwater modeling is required as part of the RFI/RI/BRA if groundwater contamination in excess of MCLs has been identified or if future groundwater contamination is imminent, as determined by the core team. The purpose of performing modeling in the RFI/RI/BRA stage of an operable unit (OU) is to identify data gaps that may exist in the characterization, predict what the plume will look like in the future, and assess the need for early action. Groundwater modeling is required only for the refined groundwater Constituents of Concern (COCs); however, modeling of other constituents may be included on the basis of parent/daughter relationships with the refined COCs, potential future threat to groundwater, etc. The following steps describe the modeling approach and documentation of the modeling effort performed during this stage of the RCRA/CERCLA process.

Step 1. Develop a Hydrogeologic Conceptual Model

The hydrogeologic conceptual model (HCM) is a simplified representation of the groundwater flow system, frequently in pictorial form that defines the hydrostratigraphic units of interest and all system boundaries. The HCM involves delineation of groundwater sources and sinks, expected flow directions, model discretization (in terms of space and time), and selection of appropriate computer code(s). The HCM and modeling code will be discussed with technical team members from each agency at an HCM meeting. The results of the HCM meeting will be presented to the core team for approval at the Post Characterization Scoping Summary meeting.

To design the model, it is necessary to specify the model type (i.e., 1D, 2D, or 3D) that best suits the objectives of modeling, the data set available, the model domain and the conditions encountered at the site. Once the model type has been specified, it is possible to discretize the model domain in time and space. One goal of model design is to simplify the system so it can be analyzed by reasonable means.

Normally, modeling performed as part of the RFI/RI/BRA shall use codes available in the Department of Defense Groundwater Modeling System (GMS). The US EPA and SCDHEC have accepted GMS for use at the SRS. When needed for special modeling tasks, SRS will obtain approval from US EPA and SCDHEC for use of other groundwater modeling codes that are not part of the GMS suite of codes. This is exclusive of parameter estimation codes used for model calibration (such as PEST or HydroFACT), or for quantifying the uncertainty in model predictions. The modeling codes to be used will be discussed at the HCM meeting and a technical recommendation will be presented to the core team for approval. The modeling lead for the respective teams have the responsibility for preparing and presenting the ER position to the core team.

Step 2. Calibrate the Model

The calibration of a groundwater flow model is the process of adjusting hydraulic parameters, boundary conditions and initial conditions within reasonable ranges to obtain a match between observed and simulated potentials, flow rates, and other calibration targets. The range over which model parameters and boundary conditions may be varied is determined by data presented in the conceptual model. In the case where parameters are well characterized by field measurements, the range over which that parameter is varied in the model should be consistent with the range observed in the field. The degree of fit between model simulations and field measurements can be quantified by statistical means. The following paragraphs describe the steps to be taken for calibration of the model.

Prior to calibration of the groundwater flow model appropriate calibration targets are selected from the available head data or other field data. The calibration criteria are then defined, providing the rationale for establishing when a model is calibrated and when calibration efforts should be terminated. The appropriate rationale for establishing acceptable quantitative calibration target residuals and residual statistics for analyzing model error (how well the model simulates the physical system) depends on several factors: the degree of natural heterogeneity or complexity of boundary conditions; location, number and accuracy of water level measurements; and the model purpose. The acceptable residual should be a small fraction of the difference between the highest and lowest heads across the site and be based on:

- The magnitude of the change in heads over the problem domain in the specific area(s) of interest;
- The ratio of the Root Mean Squared (RMS) error to the total head loss should be small;
- Head differential of <5% for the residual mean and standard deviation, and <10% for the ratio of the standard deviation to total head change.
- Krig the measured hydraulic head distribution to produce unbiased estimates of variance (standard deviation) as a function of location in the model domain.

After calibration, the coefficients of variation as well as the differences between calibrated targets and simulated heads and fluxes shall be presented in the model documentation. A modeling report shall be prepared to provide a discussion of the calibration procedure, changes in initial parameter estimates, and the sensitivity of the model to these changes.

Step 3. Perform Calibration Sensitivity Analysis

The purpose of calibration sensitivity analysis is to quantify the sensitivity of the calibrated model to changes in the estimates of aquifer and confining unit parameters, stresses and boundary conditions (i.e. the goal is to identify model inputs that have the most influence on model calibration and predictions). The magnitude in the changes in parameters should be based on estimates of uncertainty in the parameter values. During the CMS/FS process (discussed below), uncertainty analysis is performed to assess the effect of uncertainty on model predictions using the calibrated model.

At a minimum, the following parameters will be considered in the calibration sensitivity analysis: hydraulic conductivity, recharge, K_d , dispersivity, and porosity. Other inputs (such as boundary conductance or heads) that are likely to effect the computed head, groundwater flow rates and mass flux of contaminants may be varied as appropriate. The primary parameters to use in the sensitivity analysis will be discussed and decided on by the core team at the Post Characterization Scoping Summary meeting. The sensitivity of each parameter to the model solution is evaluated by looking at residuals (observed value minus the predicted

value) and calibration statistics in tabular and graphical forms (comparing objective functions and residuals vs. perturbation multipliers) and using maps with residual postings.

Step 4. Document the Modeling Effort

A stand-alone document will be prepared which documents the detailed assumptions, inputs, sensitivity analysis and evaluation of the model limitations. The Executive Summary of this document shall be written in sufficient detail, so that it can be incorporated in Chapter 6 of the RFI/RI/BRA Report.

CMS/FS Stage

In the CMS/FS stage, the groundwater model may be revised to include any new data that was collected that may aid in reducing the uncertainty in model predictions. Also, proposed remedial alternatives will be studied and compared based on the developed remedial alternatives conceptual model (RACM), as required. The RACM consists of a short summary and description of how each remedial alternative being considered in the CMS/FS will be modeled. THE RACM will also include justification for any groupings of alternatives in the modeling. The modeling of the proposed remedial alternatives will be performed in a manner similar to the steps defined above for the RFI/RI/BRA stage. Typical uses for modeling at the CMS/FS stage are to evaluate combinations of active and passive remedial alternatives, to analyze changes in plume dynamics (e.g., accelerating/retarding contaminant transport, contamination of other areas, etc.) and to predict aquifer restoration time. The remedial alternatives to be modeled will be discussed, and agreed to, by the technical team members from each agency. The results of the RACM meeting will be presented to the core team at the FS Scoping meeting.

Uncertainty associated with modeling predictions for remedial alternatives will be studied and presented in the CMS/FS. The uncertainty is a deviation between model predictions because of incomplete knowledge about head distribution, aquifer parameters and/or hydrologic stresses. Sources of uncertainty in model predictions are usually; 1) conceptual uncertainty – unsure of the physical processes occurring, 2) model derived uncertainty – the modeling approach is a simplified representation of reality, and 3) parameter uncertainty – unsure of the modeling parameter values used in the model.

The Monte Carlo Analysis approach will be used for assessing prediction sensitivity (uncertainty) analysis. Monte Carlo Analysis involves running many realizations or scenarios (random combinations of parameters) and comparing predictions or results for those realizations that are reasonable (within realistic ranges for the parameters) and remain in calibration. The parameter uncertainty, correlations (if any), expected Monte Carlo realizations, and predicted values for will be specified in the RACM for each remedial alternative.

The uncertainty will be studied for the “base case” (i.e., natural attenuation), and for each proposed remedial alternative. The results should be summarized and compared by studying calibration residuals and statistics in tabular and graphical forms. Also, the predicted values for each scenario will be summarized and compared for selected observation points within the model domain.

A stand-alone document that describes the modeling performed for the remedial alternatives will be prepared with the results being incorporated and evaluated in the CMS/FS.